

1-Naphthalenecarboxamide, N-(3-chlorophenyl)-

Inchi: InChI=1S/C17H12ClNO/c18-13-7-4-8-14(11-13)19-17(20)16-10-3-6-12-5-1-2-9-15(12)16

InchiKey: MROMMCULOKJDLK-UHFFFAOYSA-N

Formula: C17H12ClNO

SMILES: O=C(Nc1cccc(Cl)c1)c1cccc2ccccc12

Mol. weight [g/mol]: 281.74

Physical Properties

Property code	Value	Unit	Source
gf	353.01	kJ/mol	Joback Method
hf	172.13	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	78.52	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	4.745		Crippen Method
mvol	207.200	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	2658.00		NIST Webbook
rinpol	2658.00		NIST Webbook
tb	812.13	K	Joback Method
tc	1071.62	K	Joback Method
tf	524.44	K	Joback Method
vc	0.783	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.08	J/mol×K	812.13	Joback Method
cpg	561.65	J/mol×K	855.38	Joback Method
cpg	573.14	J/mol×K	898.63	Joback Method
cpg	583.69	J/mol×K	941.87	Joback Method
cpg	593.45	J/mol×K	985.12	Joback Method
cpg	602.53	J/mol×K	1028.37	Joback Method
cpg	611.10	J/mol×K	1071.62	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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